PGD-Based Advanced Nonlinear Multiparametric Regressions for Constructing Metamodels at the Scarce-Data Limit

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Overview of Advanced Regressions in Engineering Applications

- **Metamodels in Engineering:** Utilization of regressions from experimental or simulated data for various applications.
- **Multi-Parametric Physics:** Solutions applicable in real-time engineering tasks like optimization, inverse analysis, and simulation-based control.
- **Model Order Reduction (MOR):** Advanced MOR techniques for solving complex multi-parametric problems.
- **Regression-Based Solutions:** Approach for high-dimensionality challenges in limited data scenarios by creating regressions from parametric value samples.
- **Challenges:** Addressing accuracy and avoiding overfitting in high-dimensional, low-data environments.
- **PGD-Based Regressions:** Proposing and discussing advanced regressions based on Proper Generalized Decomposition (PGD) to address these challenges.

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Introduction to Advanced Regression in Model Order Reduction

- **Concept of Model Order Reduction (MOR):** MOR techniques reduce the complexity of problem solutions, such as those formulated by partial differential equations (PDEs), by representing them in a reduced basis with strong physical or mathematical significance.
- **Reduced Basis Methods:** These bases are typically derived from offline solutions using techniques like Proper Orthogonal Decomposition (POD) or the Reduced Basis Method (RB).
- **Comparison with Finite Element Method (FEM):** The reduced basis approach contrasts with FEM, where solution complexity scales with mesh size. The reduced basis size is generally much smaller, leading to significant computational savings.

Introduction to Advanced Regression in Model Order Reduction

- **Accuracy vs. Generality in MOR:** While reduced basis methods speed up computation, they might limit generality. Accuracy is maintained as long as the solution resides within the reduced basis space.
- **Proper Generalized Decomposition (PGD):** PGD constructs the reduced basis and solves the problem simultaneously, improving accuracy but increasing intrusiveness.
- **Non-Intrusive Methods:** To reduce intrusiveness, non-intrusive methods construct parametric solutions from high-fidelity solutions computed offline for different model parameters (DoE).

Introduction to Advanced Regression in Model Order Reduction

- **Challenges with High-Dimensional Data:** Addressing high-dimensionality in the low data limit poses significant challenges, including the risk of overfitting and maintaining accuracy.
- **Orthogonal Polynomial Approximations:** These approximations, despite being simple, can be highly effective but risk overfitting in high-dimensional settings. Kriging approximations are an alternative to mitigate this issue.
- **Sparse Subspace Learning (SSL) and s-PGD:** SSL interpolates pre-computed solutions across the parametric space, while s-PGD uses sparse sampling to reduce data requirements.

Introduction to Advanced Regression in Model Order Reduction

- **Regression in AI and Scientific Machine Learning:** Regressions play a crucial role in modeling physical reality, particularly important in AI applications within physical contexts.
- **Curse of Dimensionality:** In multi-parametric settings, the exponential growth in the number of required sampling points (degrees of freedom) poses significant challenges.
- **Parsimonious Models and Sparsity:** Emphasis on parsimonious (simple and sufficient) models and implementing sparsity in regression helps address the challenges of high-dimensional data.

Introduction to Advanced Regression in Model Order Reduction

- **Proposed Regression Methodologies:** The paper proposes robust, frugal, and accurate regression methodologies suitable for separated representation settings. These include Elastic Net regularized formulation (*rs*-PGD), doubly sparse regression (s^2-PGD), and ANOVA-PGD.
- **Elastic Net Regularized Formulation:** Combines Ridge and Lasso regressions to balance the need for smaller coefficients and sparsest solutions.
- **Doubly Sparse Regression and ANOVA-PGD:** These techniques aim to efficiently manage data scaling and approximation richness in high-dimensional settings.

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2 Regularized regressions: *rs*-PGD and s^2-PGD

- **Introduction:** This section introduces two novel numerical techniques: the regularized sparse PGD (*rs*-PGD) and the doubly sparse PGD (s^2-PGD).
- **Structure:** The content is organized into three subsections: theoretical background, the formulation of *rs*-PGD, and the formulation of s^2-PGD.

2.1 Theoretical background: the *s*-PGD

- **Objective Function:** The goal is to approximate an unknown function $f : \Omega \subset \mathbb{R}^d \to \mathbb{R}$, depending on d variables.
- **Sparse PGD Approach:** The sparse PGD (*s*-PGD) approximates f using a low-rank separated (tensor) representation, expressed as a sum of products of one-dimensional functions.
- **Formulation:** Each function ψ_m^k is expressed from standard approximation functions, with the choice of basis functions being crucial.
- **Regression Problem in *s*-PGD:** Focuses on minimizing the L2-norm distance to the sought function, with challenges arising in high-dimensional problems, especially with sparse data.
- **Modal Adaptivity Strategy (MAS):** Used in *s*-PGD to minimize spurious oscillations outside the training set by starting with low-degree modes and introducing higher order functions as needed.

2.2 *rs*-PGD

- **Objective:** Extend the sparse PGD to enhance predictive capacity and handle sparse identification in regression problems.
- **Formulation:** Introduces a penalty term in the regression to reduce overfitting and deal with strong multicollinearity.
- **Regularizations:** Different regularizations like Tikhonov or Elastic Net regularization can be employed.
- **Ridge Regression Regularization:** A form of Tikhonov regularization, used to illustrate the approach which will later be generalized to Elastic Net regularization.
- **Elastic Net Regularization:** Combines L1 and L2 norms to balance between penalty factors and aims for sparsity and minimization of overfitting.

2.3 s^2-PGD

- **Objective:** Focuses on identifying non-zero coefficients in each enrichment step for constructing parsimonious models.
- **L1 Regularization:** Promotes sparsity in the solution by minimizing a function involving the L1 norm.
- **Iterative Scheme:** Employs an alternate direction fixed point strategy, solving a LASSO regression problem in each dimension.
- **Model Selection:** Uses criteria like minimum sparsity and cross-validation for selecting models and penalty factors.
- **De-Biasing:** After model selection, Ordinary Least Squares (OLS) methodology is employed to correct the bias introduced by LASSO regression.

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3 The ANOVA-based Sparse-PGD

- **Introduction:** Discusses ANOVA decomposition for a function $f\left(s^1, \ldots, s^d\right)$ and its application in sparse-PGD.
- **ANOVA Decomposition:** Presents the function as a sum of orthogonal functions, capturing different variable interactions.
- **Orthogonality:** Emphasizes the orthogonality of functions in the decomposition, essential for the statistical modeling aspect of ANOVA.

3.1 Sensitivity Analysis: Sobol Coefficients

- **Variance Analysis:** Explores the variance of $f(\vec{s})$ based on the orthogonality in ANOVA decomposition.
- **Sobol Sensitivity Coefficients:** Introduces Sobol coefficients $\mathcal{S}_n$ which quantify the contribution of each component in the decomposition to the overall variance.

3.2 The Anchored ANOVA

- **Computational Challenges:** Addresses the computational difficulties in multidimensional expectations in ANOVA.
- **Anchor Point Concept:** Introduces an anchor point $\vec{c}$ to simplify the computation of multidimensional expectations.
- **Adapted Decomposition:** Describes how the functions in ANOVA decomposition are modified using the anchor point for efficient computation.

3.3 Combining the Anchored-ANOVA with the Sparse PGD

- **Strategic Approach:** Proposes a strategy combining anchored-ANOVA and sparse PGD for efficient function approximation.
- **Initial Evaluation:** Uses anchored-ANOVA for evaluating functions dependent on each dimension.
- **Residual Computation:** Details the process of computing the residual function $f'(\vec{s})$.
- **Application of Sparse PGD:** Suggests using *rs*-PGD or s^2-PGD for approximating the residual, incorporating enhanced sparse-sampling.

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4 Results

- **Overview:** Presentation of results using *rs*-PGD, s^2-PGD, and ANOVA-PGD in different cases.
- **Error Reduction:** Comparison of error reduction in *rs*-PGD compared to classical *s*-PGD.
- **Sparse Identification:** Examination of sparse identification and error reduction using s^2-PGD compared to standard *s*-PGD.
- **ANOVA-PGD Methodology:** Analysis of variance combined with regularized approximations for advanced regression methods.

4.1 Results for the *rs*-PGD Approach

- **Elastic Net Regularization:** Utilization of the α parameter to combine Ridge and Lasso regression for predictive performance optimization.
- **Five-Dimensional Polynomial Example:** Significant error reduction observed in a complex polynomial case using *rs*-PGD with specific α settings.
- **Trigonometric and Logarithmic Functions:** Application of *rs*-PGD in a multifaceted function, achieving considerable error reduction.
- **Chaotic Lorenz System:** Successful detection of non-zero coefficients in a chaotic system with minimal error, utilizing ridge regularization and MAS.

4.2 Checking the Performances of s^2-PGD

- **Sparsity in One Dimension:** Examination of a function involving sine, Chebyshev polynomial, and exponential terms, showing significant improvement in predictions with s^2-PGD.
- **More Dimensions Example:** In a complex multidimensional function, the s^2-PGD accurately identifies non-zero elements, greatly reducing error compared to standard s-PGD.

4.3 ANOVA-PGD Numerical Results

- **ANOVA-PGD Regression:** Application of regression techniques to various terms in ANOVA decomposition, highlighting the benefits of orthogonality and low-dimensional settings.
- **2D Function Example:** Application to a 2D function with complex terms, showing the effectiveness of ANOVA-based regression compared to standard *s*-PGD.

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5 Conclusions

- **Introduction of Techniques:** Highlighting the introduction of three advanced data-driven regression techniques: *rs*-PGD, s^2-PGD, and ANOVA combined with sparse separated representations.
- **Improvement Over Sparse *s*-PGD:** Discussing the significant improvements these techniques bring to the sparse *s*-PGD, especially in reducing overfitting and enhancing predictive capabilities.

Advancements in Regression Techniques

- **Sparse Identification and Variable Selection:** Emphasizing the ability of s^2-PGD to identify sparsity and select variables effectively, particularly where s-PGD falls short.
- **Examples of Improvement:** Referencing specific examples (Figures 7 and 8) that demonstrate the substantial improvements made by these new methods.

Future Prospects and Industrial Applications

- **High-Performance ROMs:** Discussing the potential of these techniques in constructing high-performance Reduced Order Models (ROMs) in challenging low-data, high-dimensional contexts.
- **Industrial Interest:** Addressing the growing industrial interest in obtaining accurate models under these challenging conditions.
- **Ongoing and Future Work:** Mentioning ongoing work in specific industrial applications and exploring additional penalties and sampling strategies to maximize ROM performance.

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Overview

- This section compares Physics-Informed Neural Networks (PINNs) with sparse PGD-based techniques like s-PGD, rs-PGD, and s^2-PGD.
- Focuses on the advantages and disadvantages of PINNs in contrast to these techniques.

Advantages of PINNs

- Integration of Physical Laws into Learning
- Flexibility in Handling Complex Geometries and Boundary Conditions
- Data Efficiency in Scenarios with Limited Data
- Adaptability to Different Types of PDEs and Scenarios
- Benefits from Advancements in Deep Learning (e.g., GPU acceleration)

Disadvantages of PINNs

- High Computational Cost for Training
- Sensitivity to Hyperparameters
- Lack of Interpretability Compared to Traditional Methods
- Requirement for Well-Defined Physical Models
- Challenges in Numerical Stability and Accuracy

Comparison with Sparse PGD-based Techniques

- Model Complexity: Less complex in sparse PGD-based methods.
- Data Requirement: PINNs are more flexible with unstructured data.
- Physical Constraints Integration: More inherent in PINNs.
- Computational Efficiency: Sparse PGD methods may be more efficient for well-established problems.
- Ease of Use: Sparse PGD methods are more straightforward for traditional computational method users.

Conclusion: Application to RANS Equations

- In the context of RANS equations for turbulent flow, the choice between PINNs and sparse PGD-based methods depends on specific requirements.
- PINNs can offer enhanced capabilities in modeling complex turbulence behaviors and interactions, particularly in high-dimensional scenarios.
- Sparse PGD methods might provide more straightforward solutions for well-established RANS problems, especially in scenarios where computational efficiency is paramount.
- Future advancements in both areas could further refine their applicability to RANS equations, balancing accuracy, computational cost, and physical fidelity.